Vertical and Diagonal Stripes in the Extended Hubbard Model

M. Raczkowski[1]) (a), B. Normand (b), and A. M. Oleś (a)

(a) Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland
(b) Département de Physique, Université de Fribourg, CH-1700 Fribourg, Switzerland

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Abstract

We extend previous real–space Hartree–Fock studies of static stripe stability to determine the phase diagram of the Hubbard model with anisotropic nearest–neighbor hopping t, by varying the on–site Coulomb repulsion U and investigating locally stable structures for representative hole doping levels $x = 1/8$ and $x = 1/6$. We also report the changes in stability of these stripes in the extended Hubbard model due to next–neighbor hopping t' and to a nearest–neighbor Coulomb interaction V.

Charge localization and the tendency of doped holes towards self–organization into striped patterns, observed in high-T_c superconductors, is one of the most interesting current topics in the physics of strongly correlated electron systems [1]. The stripe instability was predicted on the basis of mean–field calculations before their experimental confirmation, in both three–band [2] and one–band Hubbard models [3]. These calculations yielded solutions with a phase separation which is manifest in the formation nonmagnetic lines of holes, one–dimensional domain walls or stripes, which separate antiferromagnetic (AF) domains of opposite phases. These phenomena are the most pronounced in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ around hole doping $x = 1/8$ [4], where the stripes are aligned along the two lattice directions x and y, to which we refer as horizontal stripes (HS) or vertical stripes (VS). This is in contrast to the diagonal stripes (DS) inferred in the insulating nickelates $La_{2-x}Sr_xNiO_{4+y}$. However, although the multiband Hartree-Fock (HF) calculations of Zaanen and Littlewood [5] are consistent with the observation of filled stripes in nickelates, by which is meant one doped hole per stripe site, the HF approximation does not predict the half–filled stripes (one hole every two atoms) observed in cuprates [6]. In addition, charge transport in idealized stripes is not possible for the filled case. Both of these considerations indicate that it is necessary to go beyond the HF treatment of stripes by including local electron correlations which further influence the charge and spin distributions. However, significant qualitative statements remain possible within the framework of unrestricted HF.

In this paper we attempt a systematic investigation of the properties and relative stability of filled VS and DS. We use the extended single–band Hubbard model, which is widely accepted as the generic model for a microscopic description of cuprate and nickelate systems,

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle} n_i n_j, \tag{1}$$

where the operator $c^{\dagger}_{i\sigma}$ ($c_{j\sigma}$) creates (annihilates) an electron with spin σ on lattice site i (j), and $n_i = c^{\dagger}_{i\uparrow} c_{i\uparrow} + c^{\dagger}_{i\downarrow} c_{i\downarrow}$ gives the electron density. The hopping t_{ij} is t for nearest neighbors

[1]) Corresponding author; e-mail: marcin@alphetna.if.uj.edu.pl

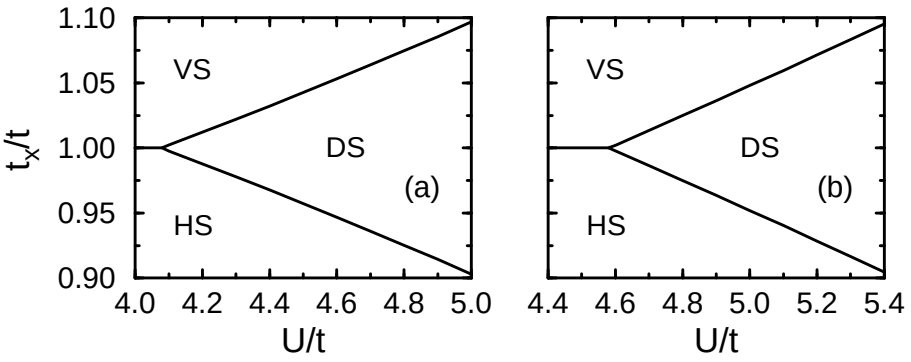

Figure 1: Phase diagrams for stable stripe structures obtained in the anisotropic Hubbard model ($t' = 0$, $V = 0$) for doping $x = 1/8$ (a) and $x = 1/6$ (b).

and t' for second–neighbor sites i and j, while the on–site and nearest–neighbor Coulomb interactions are respectively U and V. The model is solved self-consistently in real space within the HF approximation, where the interactions are decoupled into products of one–particle terms, and we focus on the representative hole doping levels $x = 1/8$ and $x = 1/6$. We do not consider noncollinear spin configurations, and use the most straightforward version of the HF method with a product of two separate Slater determinants for up and down spins, whence $n_{i\uparrow}n_{i\downarrow} \simeq n_{i\uparrow}\langle n_{i\downarrow}\rangle + \langle n_{i\uparrow}\rangle n_{i\downarrow} - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle$. A similar decoupling is performed for the nearest–neighbor Coulomb interaction. Calculations were performed on 12×12 (16×16) clusters for $x = 1/6$ ($x = 1/8$) with periodic boundary conditions, and we obtain stable stripe structures with AF domains of width five atoms for $x = 1/6$ and seven atoms for $x = 1/8$.

We begin by setting $t' = 0$ and $V = 0$. The phase diagrams shown in Fig. 1 were determined by varying U and the ratio t_x/t_y of the nearest–neighbor hoppings in the x– and y–directions, while maintaining constant $t = \frac{1}{2}(t_x + t_y)$. We observe the generic crossover from VS to DS with increasing Coulomb interaction reported in early HF studies [3]. The transition from VS to DS appears in the isotropic case at $U/t \simeq 4.1$ for $x = 1/8$ [Fig. 1(a)], and at the higher value $U/t \simeq 4.6$ for $x = 1/6$ [Fig. 1(b)]. The results have a simple physical interpretation. Stripe phases occur as a compromise between on the one hand the AF interactions among magnetic ions and the Coulomb interactions which favor charge localization, and on the

Table 1: Site–normalized local charge density $n_{\mathrm{h}i} = \langle 1 - (n_{i\uparrow} + n_{i\downarrow})\rangle$, local magnetization density $m_i^z = \frac{1}{2}|\langle n_{i\uparrow} - n_{i\downarrow}\rangle|$, and kinetic energy contributions $E_{\mathrm{K}}^{x_i}$ and $E_{\mathrm{K}}^{y_i}$ on bonds between inequivalent atoms, all labeled by decreasing doped hole density in the x–direction, for VS (left) and DS (right) in the isotropic Hubbard model ($t_x = t_y$, $t' = 0$, $V = 0$) on a 16×16 cluster with $U = 5$ and $x = 1/8$. In parenthesis are given the values of $n_{\mathrm{h}i}$ for the extended hopping model with $t'/t = -0.1$.

$n_{\mathrm{h}i}$	m_i^z	$E_{\mathrm{K}}^{x_i}/t$	$E_{\mathrm{K}}^{y_i}/t$	$n_{\mathrm{h}i}$	m_i^z	$E_{\mathrm{K}}^{x_i}/t$	$E_{\mathrm{K}}^{y_i}/t$
0.364 (0.373)	0.000	−0.844	−0.643	0.388 (0.400)	0.000	−0.722	−0.722
0.234 (0.235)	0.222	−0.662	−0.632	0.193 (0.195)	0.262	−0.624	−0.722
0.067 (0.062)	0.348	−0.600	−0.612	0.070 (0.067)	0.352	−0.606	−0.624
0.014 (0.013)	0.381	−0.595	−0.597	0.032 (0.029)	0.372	−0.596	−0.606
0.006 (0.006)	0.384	−0.595	−0.593	0.020 (0.019)	0.380	−0.596	−0.596

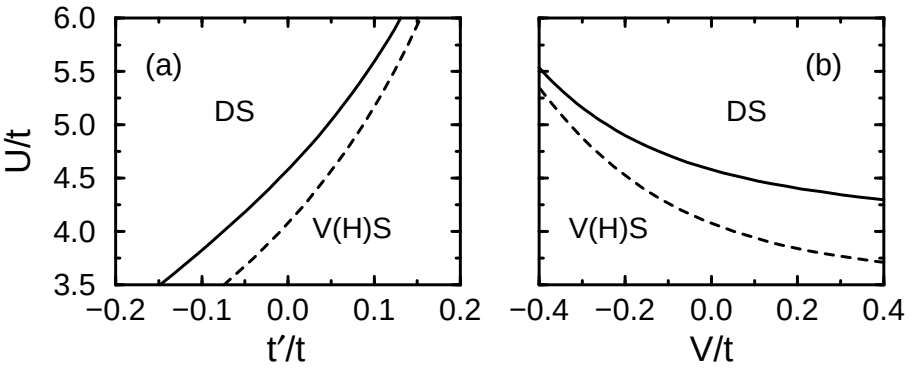

Figure 2: Phase boundaries for stripes in the isotropic extended Hubbard model with (a) $V = 0$ and (b) $t' = 0$, for dopings $x = 1/8$ (dashed line) and $x = 1/6$ (solid line).

other the kinetic energy of doped holes which favors charge delocalization. Further, previous HF studies have clarified that the largest kinetic energy gains are obtained due to hopping perpendicular to the stripes [6]. These features are seen in Tables 1 and 2. For VS one finds a large anisotropy in the values of the kinetic energies, $E_{\rm K}^{x_i}$ and $E_{\rm K}^{y_i}$, projected on the bonds in the x– and y–directions, which becomes especially pronounced beside the stripes, and is strongly reinforced by the hopping anisotropy [7]. Thus, VS always lie along the direction of weaker hopping amplitude in the anisotropic model (Fig. 1).

The kinetic energies in Table 2 show further that VS are more favorable for charge dynamics. This result, which is not immediately obvious, is due to the greater overall width of the stripe (Table 1), indicating that stripe fluctuations occur more readily in this geometry. This explains their stability at small U where the consequent cost in potential energy E_U becomes less relevant. By contrast, DS have narrower stripes with larger magetization densities m_i^z (Table 1), meaning a lower net double occupancy and hence a more favorable E_U (Table 2). The transition from VS to DS with increasing U is thus clarified.

Table 2: Site–normalized ground–state energy $E_{\rm tot}$, kinetic energy ($E_{\rm K}^x, E_{\rm K}^y, E_{\rm K}^{x-y}, E_{\rm K}^{x+y}$), and potential energy (E_U, E_V) components of VS (rows 1-5) and DS (rows 6-10) in the isotropic extended Hubbard model on a 16×16 cluster with $U = 5$ and $x = 1/8$. The DS is oriented along the direction $x - y$.

t'/t	V/t	$E_{\rm K}^x/t$	$E_{\rm K}^y/t$	$E_{\rm K}^{x-y}/t$	$E_{\rm K}^{x+y}/t$	E_U/t	E_V/t	$E_{\rm tot}/t$
0.0	0.0	−0.6753	−0.6147	0.0000	0.0000	0.4900	0.0000	−0.8000
−0.1	0.0	−0.6838	−0.5977	0.0097	0.0097	0.4821	0.0000	−0.7800
0.1	0.0	−0.6660	−0.6300	−0.0110	−0.0110	0.4968	0.0000	−0.8212
0.0	−0.4	−0.6655	−0.6083	0.0000	0.0000	0.4749	−0.6251	−1.4240
0.0	0.4	−0.6838	−0.6214	0.0000	0.0000	0.5063	0.6207	−0.1782
0.0	0.0	−0.6368	−0.6368	0.0000	0.0000	0.4696	0.0000	−0.8040
−0.1	0.0	−0.6309	−0.6309	0.0000	0.0136	0.4587	0.0000	−0.7895
0.1	0.0	−0.6417	−0.6417	0.0000	−0.0178	0.4802	0.0000	−0.8210
0.0	−0.4	−0.6319	−0.6319	0.0000	0.0000	0.4602	−0.6193	−1.4229
0.0	0.4	−0.6412	−0.6412	0.0000	0.0000	0.4789	0.6171	−0.1864

We have also considered the effect of a next–neighbor hopping t' on the relative stability of V(H)S and DS. Fig. 2(a) shows that a negative t' ($t'/t < 0$), as obtained for the realistic parameters of high–T_c superconductors, stabilizes DS [8], whereas a positive t' favors VS, within the parameter range where t' does not drive a stripe melting [8]. The explanation is contained in Table 2: negative t' gives a positive kinetic energy contribution, which is much more readily minimized by the DS charge configuration. One observes further that positive t' reduces the anisotropy between kinetic–energy gains in the x– and y–directions for VS, and makes their sum more favorable, while negative t' has the opposite effect. For DS the total kinetic energy also follows the same trend. The explanation for these results can be found in the reinforcement of stripe order by negative t' (values in parenthesis in Table 1), which suppresses the hopping contributions, and its smearing out by positive t' where hopping is enhanced. These trends agree with the earlier finding within the dynamical mean field theory that VS are destabilized by kink fluctuations [9]. However, this stripe (dis)ordering tendency also leads to a considerably greater change in the Coulomb energy E_U for DS than for VS (Table 2), best seen in the charge–density alterations within the stripes (Table 1), which contributes significantly to the predominance of DS for negative t'.

Finally, we investigate the changes in stripe stability due to repulsive ($V > 0$) and attractive ($V < 0$) nearest–neighbor Coulomb interactions, which give the phase boundaries between VS and DS shown in Fig. 2(b). Attractive V enhances VS stability, while repulsive V favors DS. The tendency towards VS formation at $V < 0$ is due primarily to their much higher charge densities on nearest-neighbor sites along the stripe, a situation which is avoided by DS (Table 2). While this is also the leading mechanism for VS suppression at $V > 0$, the asymmetry of the curve in Fig. 2(b) arises from the fact that the lower U values at the transition favor the higher kinetic energy contributions available for VS (above).

In summary, we have shown that a competition between vertical (horizontal) and diagonal stripes dominates the behavior of the charge structures formed on doping the Hubbard model in the physically interesting regime of $3.5 \leq U/t \leq 6$ within the HF approximation. The detailed charge distribution and the stripe ordering depend on the ratio U/t, on the value of the next–neighbor hopping t', and on the nearest–neighbor Coulomb interaction V. Both repulsive V and negative t', which correspond to the realistic parameters of high–T_c superconductors, act to reduce the relative stability of vertical (horizontal) stripes.

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